Integrated Analysis and Simulation Software Tools for Calibration and Validation of Crystal-Scale Material Models

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Novel diffraction-based methods for experimental mechanics are providing unprecedented levels of detail in the coevolution of microstructure and micromechanical state in deforming crystalline materials, such as structural metals, ceramics, and rock. Engineers at LLNL are concurrently working on novel constitutive models and simulation frameworks with increasing levels of physical detail, advancing the state of computational mechanics. There is, however, a dearth of fundamental software tools suitable for integrating experimental and simulated data. Of the few tools that exist, most were generated on *ad hoc* bases and lack the robustness and modularity necessary to make them more widely applicable and accessible to new users. This hampers critical validation and verification procedures for advanced material models, as well as collaborations seeking to leverage LLNL simulation codes. The goal of this project is to bridge this gap by producing an open-source software toolkit for reducing and analyzing data from both experiments and simulations.

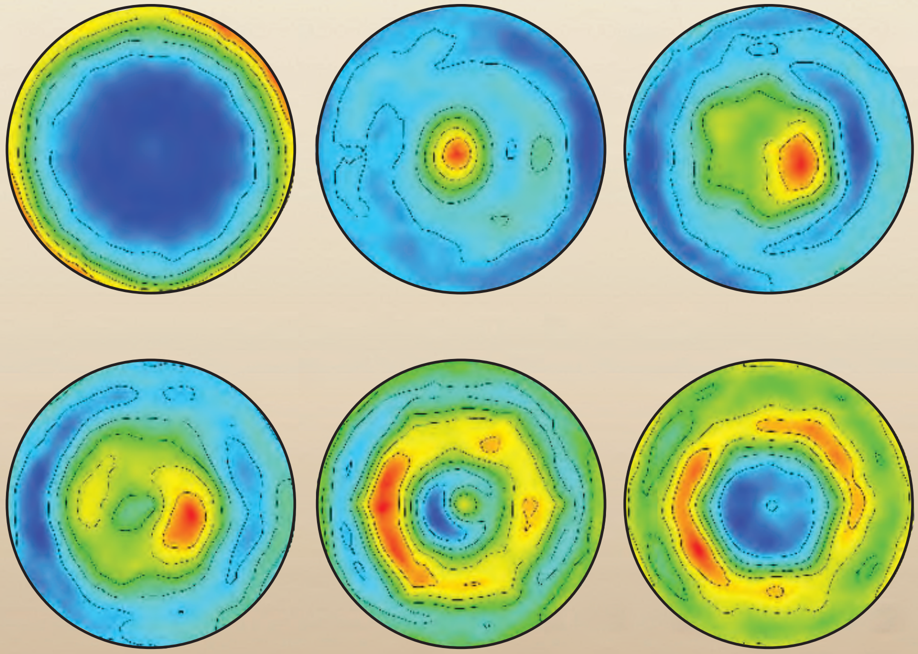

Figure 1. Reconstructed pole figures for a specimen of magnesium alloy AZ31 prior to an *in situ* deformation experiment. The underlying orientation distribution function was obtained by inverting experimental data onto a finite element mesh over the orientation space. The indices by row from the top left are: {001}, {100}, {110}, {111}, {112}, {113}. The color map indicates multiples of the uniform distribution with blue at 0 and red at 3; this normalization implies that the mean value of each pole figure is unity.

Project Goals

This project is a continuation of an FY2008 effort that focused on producing the core software library. The functionalities include:

1. Experimental diffraction data reduction for flat panel detectors:
   a. Calibration;
   b. Lattice strain extraction;
   c. Pole figure inversion (quantitative texture analysis); and
   d. Strain pole figure inversion (quantitative strain/stress analysis).
2. Simulation data reduction:
   a. Data extraction from ALE3D;
   b. Discrete orientation distributions (quantitative texture analysis); and
   c. Lattice strain/stress distributions (strain partitioning/localization, phase transformations).
3. Material Point Simulator (MPS): lightweight material model evaluation using mean field theories.
4. Model parameter optimization: general harness for running the MPS or ALE3D within a nonlinear optimization framework.

The goals of the FY2009 effort were twofold: 1) to produce user interfaces for calibrating flat panel detectors (as used at synchrotron user facilities), running the MPS, and viewing pole figures and orientation distribution functions; and 2) to refine the core software routines based on user feedback. This software has been released for unlimited distribution.

Relevance to LLNL Mission

This contribution supports ongoing work under LLNL's Engineering Simulation and Measurement Technology Roadmaps. Specifically, this software toolkit will supplement simulation efforts toward understanding the fracture and strength of metals, as well as experimental characterization of relevant microstructural features, such as orientation distributions and intergranular stresses. In addition, the software will benefit users of materials science beamlines at synchrotron user facilities throughout the DOE complex, such as at the Advanced Light Source at Lawrence Berkeley National Laboratory, and the Advanced Photon Source at Argonne National Laboratory. Clear, simple interfaces, graphical where applicable, are critical to the accessibility and utility of this toolkit.

FY2009 Accomplishments and Results

We are able to exercise material models using the MPS as well as ALE3D, extract the relevant history variables, and create data metrics such as orientation distributions, which are readily comparable to experimental results. The user interface provides graphical output as the simulation runs, updating any number of specified responses such as stress-strain response, pole figures, and phase/twin volume fractions.

Figure 1 shows screenshots of the basal plane pole figure, stress-strain time history, and twin volume fraction time history for a virtual magnesium sample subject to uniaxial compression. Similar distributions can be constructed from experimental data, which may in turn be used to verify the model performance. A framework for parameter optimization using the MPS is provided as well.

The software toolkit produced under this project comprises a library of core routines that facilitate several fundamental data visualization analysis tasks, including simple graphical user interfaces suitable for non-expert users.

Figure 2 shows calibration results for an elasto-viscoplastic constitutive model for magnesium.

Related References

1. Bernier, J. V., M. P. Miller, and D. E. Boyce, *J. Appl. Cryst.,* **39**, pp. 697–713, 2006.
2. Barton, N. R., J. V. Bernier, and J. K. Edmiston, *Proceedings of the 9th Conference of the American Physical Society Topical Group on Shock Compression in Condensed Matter*, pp. 73–78, 2009.

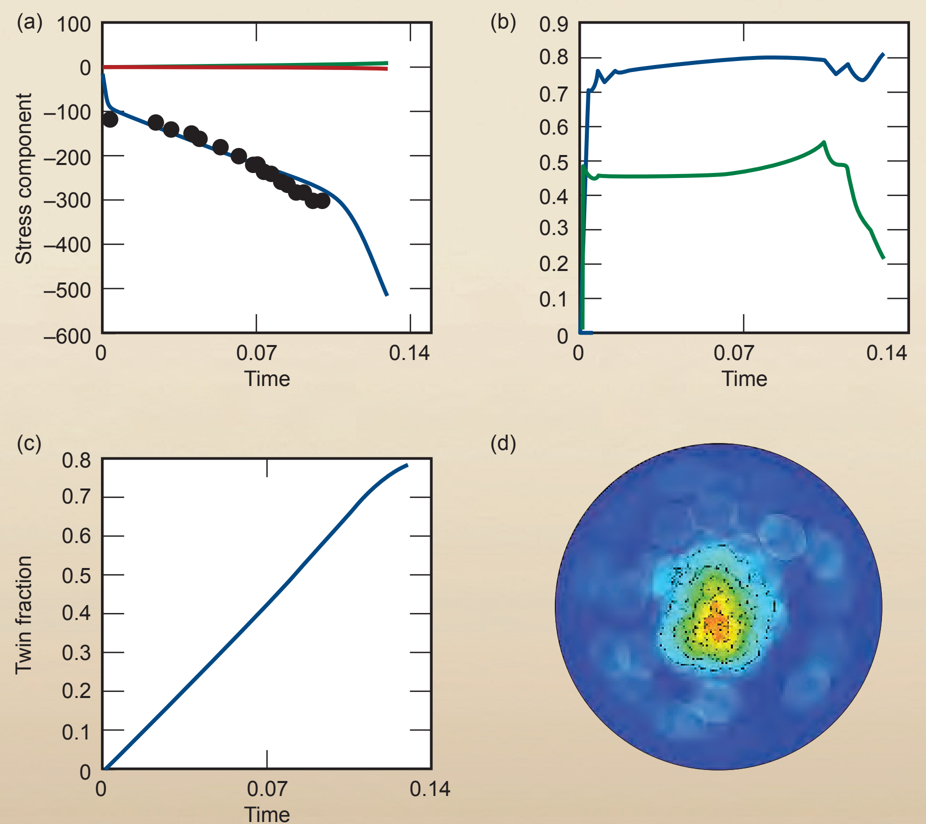

Figure 2. Calibration results for an elasto-viscoplastic constitutive model for magnesium that captures the {1012} <1011> twinning mechanism using the material point simulator. An aggregate of 1302 crystals representing the preferred orientation described by the pole figures in Fig. 1 was subject to uniaxial compression using a Taylor linking assumption (uniform deformation rate). (a) Aggregate averaged normal stress components (red and green are perpendicular to the compression axis; blue is parallel). The black points represent experimental data. (b) Decreases in effective plastic deformation rate. (c) Evolution of twin volume fraction with deformation. (d) Simulated basal {001} plane pole figure using the same scale as in Fig. 1.